UNITED STATES ENVIRONMENTAL PROTECTION AGENCY REGION 8

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Geochemical Model Acceptance Criteria Checklist for the Dewey-Burdock Project

Prepared in support of the Underground Injection Control Class III Area Permit for the Dewey Burdock Uranium In-Situ Recovery Project,

Custer and Fall River Counties, South Dakota

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Geochemical Model Acceptance Criteria Checklist for the Dewey-Burdock Project

The purpose of this checklist is to provide considerations for the evaluation and acceptance of a geochemical model with reactive transport for the Dewey-Burdock project site. This checklist accompanies and reflects discussions and considerations in the *Draft Criteria for Development of a Geochemical Model of the Dewey Burdock Project* and the *Draft Geochemical Model Criteria Support Document for the Dewey-Burdock Project*. This checklist is based on a criteria checklist in Newman (2018), with additional content added to tailor the checklist to reflect the needs of the development of the Underground Injection Control (UIC) Class III permit for the Dewey-Burdock site.

Category	Consideration	Response	Notes
	Do the capabilities of the modeling program meet the project needs in terms of hydrogeologic and geochemical capabilities?		
	Are the limitations of the geochemical modeling program clearly stated?		
	Are any simplifying assumptions that will affect the modeling results described and justified?		
General Model Considerations	How well is the choice of model supported by the quantity and quality of available data?		
	How closely does the model approximate the real system of interest (i.e., the Dewey-Burdock site)?		
	Are there factors or events that might trigger the need for major model revisions or circumstances that might prompt users to seek an alternative model?		
General Project	Have quality assurance (QA) procedures for sampling, sample handling, and analysis been set up, clearly defined, and followed?		
Quality Assurance	Does the model perform the specified task while meeting the objectives set by QA project planning?		
Model Grid and Time Steps	Does the areal extent of the model domain encompass the following areas of the project site?		

Category	Consideration	Response	Notes
	Area upgradient of the extraction zone;		
	All ore bodies;		
	Area downgradient of the extraction zone; and		
	Margin beyond the aquifer exemption boundary.		
	Does the model grid represent the injection and production wells consistently with planned operations?		
	Does the domain include a margin that is sufficiently extensive in all directions around the project site to minimize the effects of uncertainty in boundary conditions on the modeling results? Is the rationale for margins explained?		
	Does the grid spacing provide the appropriate resolution for the scale of the geochemical processes, fluid mixing, and groundwater flow patterns in the extraction area (e.g., relative to the scale of the fivespot patterns)?		
	Are the time steps appropriate for representing the geochemical processes at the site?		
	Did the model test the effects of various time steps to ensure that simulations capture the scale of geochemical processes at the site?		
Duration of	Does the model cover a sufficient timeframe, (i.e., through the post- restoration phase and through the reestablishment of natural groundwater flow) to simulate potential rebound release of uranium and other metals?		
Simulation	Is the justification for the selected timeframe clearly explained?		
	Does the model account for consecutive/concurrent injection and restoration cycles?		
Representation of Geologic and Hydrogeologic Features	Does the layering in the model domain (or other representation in 1-D or 2-D reactive transport) represent the ore formation (the Inyan Kara, including the Chilson Member, Fuson Shale, and Fall River), the confining zones (Graneros Group and Morrison Formation), and other underground sources of drinking water (USDWs) in the project area?		

Category	Consideration	Response	Notes
	Are the representations of these formations consistent with available field-based data regarding thickness, depths, dip, lenses, etc.?		
	Does the model accurately capture differences in characteristics (including lithology, mineralogy, and geochemistry) between the Dewey and Burdock areas of the site?		
	Are gaps in field-based data noted? What limitations do they pose for the modeling?		
	Do the hydrogeologic properties (porosity, permeability, etc.) assigned to the lithologies in the model domain agree with available data? Are inconsistencies (e.g., between lab and core data) identified and discussed and the selected model assumptions justified?		
	How are variability and local heterogeneity in properties (e.g., porosity, permeability) handled in the model? Are average properties used, or was a distribution developed? If so, was the process for developing the distribution described?		
	Are graphics provided showing the domain and how lithologies and properties are distributed in the grid?		
	Are all artificial penetrations represented?		
	Are geochemical boundary conditions (e.g., gas partial pressures, mineral phases, concentration boundaries) reasonable for the objectives of the model and consistent with available data? Do the data include the most recent information available? Are limitations or data gaps noted?		
Boundary Conditions	Are hydrogeologic boundary conditions of the model reasonable for the objectives of the study and consistent with available data? Do the data include the most recent information available? Are limitations or data gaps noted?		
	Are the boundary conditions of the model defined such that they do not overly constrain the model results and the calibration is appropriately sensitive and predictions are realistic?		

Category	Consideration	Response	Notes
	Are the geochemical initial conditions (e.g., groundwater chemistry, mineral assemblages) based on a sufficient number of adequate, high-quality data points? Do the data include the most recent information available? Are limitations or data gaps noted?		
	Do the background groundwater quality data represent the site, both temporally and spatially? How recently were data collected? Are data gaps identified?		
Initial Conditions	Are the hydrogeological initial conditions (e.g., groundwater flow, head distributions) based on adequate data? Do the data include the most recent information available? Are limitations or data gaps noted?		
	Are redox conditions defined throughout the project site?		
	Are differences between the Dewey and Burdock areas of the site represented?		
	Are geochemical processes modeled that are representative of the activities and types of fluid-rock interactions expected at the Dewey-Burdock site during the project life cycle? These include:		
	Interactions between the lixiviant and the ore zone groundwater and solids during <i>in-situ recovery</i> (ISR) operations;		
	Interactions between the post-ISR solids and the restoration fluid;		
Modeled Species and Processes	Interactions between the post-restoration sediments and the upgradient groundwater that moves into the restored zone;		
	Interactions between downgradient solids and the initial slug of restored groundwater that moves downgradient; and		
	Interactions between the downgradient solids and the upgradient groundwater that has passed through the restored extraction zone.		
	Do the modeled processes account for and address mechanisms by which uranium and other metals could be mobilized after restoration?		

Category	Consideration	Response	Notes
	Was the potential for colloid-facilitated transport of uranium and other metals considered?		
	Do the modeled processes reflect differences in mineralogy and other characteristics between the Dewey and Burdock sites?		
	Do the model inputs specify species and reactions that include constituents of concern with maximum contaminant levels (MCL)s or alternate concentration limits (ACLs)? (See Table 2 in the conceptual site model (CSM) support document.)		
	Are the minerals specified for modeling inputs consistent with mineralogic analyses based on field data? Do they represent the upgradient, ore zone, and downgradient regions of the project site? Do they represent oxidation state of uranium, iron, manganese, and other redox-sensitive metals in the solids? Are iron phases in the sediment characterized appropriately?		
	Are the geochemical processes specified in the model consistent with available groundwater chemistry and solids data? (For example, are mass transfer reactions (dissolution and precipitation) consistent with observed solids mineralogy? Are ternary aqueous calcium-uranyl-carbonate complexes included?)		
	Is local equilibrium being assumed? If so, is this justified?		
	Which processes are governed by kinetics? Are these selections discussed?		
	Were laboratory experimental data for sorption and leaching used to confirm that the correct reactions are being modeled, and were the data analysis procedures for experimental results described?		
	Does the thermodynamic database include the aqueous species, surfaces, and complexes likely to be important in the system?		
	Are edits made to the existing thermodynamics databases used for the evaluation specified?		
	Are the thermodynamic data for uranium and other trace metals the most currently available?		

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	Is the activity coefficient model selected appropriate for the ionic strength of the fluid and the species being modeled?		
	Which data are used for kinetic parameters? If an existing kinetics database was updated or augmented, is this identified and explained? Are the rate laws for new parameters being added consistent with the rate laws in the model?		
	Do the water quality analyses available for model inputs include constituents with primary or secondary drinking water standards or ACLs? (See Table 2 in CSM support document.)		
	Are the water quality analyses of acceptable quality according to the project QA requirements?		
	Were groundwater samples analyzed for a comprehensive suite of analytes, and are these all incorporated into the model? (See Table 2 in the CSM support document.)		
	Was the content of organic matter in sediments measured?		
Water Quality Data and Solids	Were appropriate field measurements taken (e.g., pH, T, Eh) and used in the modeling?		
Geochemical Data	Is the charge balance for water quality analyses off by <10% and if not, has this been addressed?		
	Have the water quality data been vetted for potential outliers based on historical or other data?		
	Do the water quality data spatially represent the sites necessary to simulate geochemical processes at the site, including upgradient, ore body, and downgradient to the aquifer exemption boundary?		
	If analytes are proposed to be either not analyzed or their monitoring discontinued, is this supported by existing data and is it likely to affect modeling results?		
	Were sufficient rounds of baseline sampling data collected, both temporally and spatially? How recently were data collected? Are data gaps identified?		

Category	Consideration	Response	Notes
	After the initiation of the extraction, restoration, and post-restoration phases, will monitoring data be used to update the CSM and the geochemical model?		
	Were the effects of microbial populations considered, including their potential to affect uranium recovery or establish reducing conditions after restoration?		
	Are the parameters that were calibrated clearly identified and justified?		
	Were laboratory experimental data for sorption and leaching used to parameterize the model? If so, were the data analysis procedures described? How were the data scaled up to field scale?		
	Was calibration done by manual or automated methods? Is the approach discussed and justified?		
	What performance measures were employed (e.g., sum-of-squares weighted residual, root mean squared weighted error, mean percentage error, coefficient of determination)?		
Model Calibration	What are the acceptability guidelines for the selected performance measures?		
	For model updates, are the quantity, quality, and limitations of field monitoring data used in inverse modeling described?		
	What approaches were used to minimize the difference between model simulations and experimental data or field data?		
	What is the difference between the simulated and actual data? Are acceptability guidelines achieved for the selected performance measures? Are there options for reducing error?		
	Are errors randomly distributed, or is there systematic bias within the model domain (when using field data)?		
Sensitivity Analysis and	Has a quantitative or qualitative assessment of uncertainty been made?		

Category	Consideration	Response	Notes
Assessment of Uncertainty	Are the sources of uncertainty discussed? Have considerations (e.g., associated with testing and monitoring plans), been made to reduce or compensate for uncertainty?		
	Have alternate Conceptual Site Models been considered where data are lacking or uncertain?		
	Has the sensitivity analysis addressed the factors likely to affect model results?		
	Do the variables or parameters tested make sense based on previous experience at the site and known factors controlling the geochemistry at a uranium ISR site?		
	Were the variables or parameters changed by amounts that reflect background variability? Were they changed by amounts that reflect anticipated future variability?		
	Does the variability used for sensitivity analyses incorporate uncertainty from all relevant sources (e.g., site-specific measurements, laboratory analyses, database and modeling-related)?		
	Were variables or parameters changed one at a time or globally? Was this decision discussed?		
	Have suggestions to reduce uncertainty in future models been included, such as the following?		
	Identifying the range and probability distribution of each model parameter;		
	Generating alternative sets of parameter values;		
	Calculating model outputs under alternative parameter sets; and		
	Assessing the influence and relative importance of each parameter from model outputs.		

Acronyms

ACL – Alternate concentration limit

CSM - Conceptual site model

ISR – *In-situ* recovery

MCL – Maximum contaminant level

QA – Quality assurance

UIC – Underground Injection Control

USDW – Underground source of drinking water